

Describing the optical properties of astronomical dust analogs through numerical techniques

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Introduction
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Modeling
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Results
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Summary
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Outline



Introduction

- The interstellar medium in the infrared
- The quest for the optical constants



1.1 Introduction

- Previous work
- Methodology



1.2 Modeling

- Experimental data and apparatus
- Analytical portraits



1.3 Results

- Conclusions
- Future perspectives

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The relation between dust and the infrared

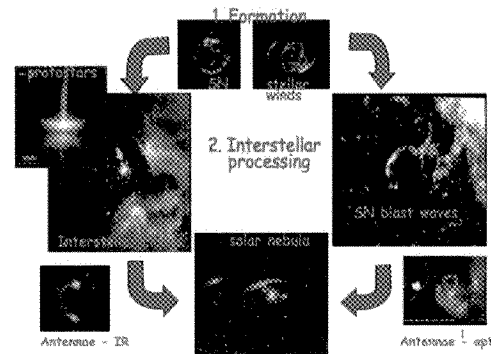


Figure: Formation, processing, and evolution of interstellar dust (Rinehart et al., 2008)

Interstellar dust:

- plays a role in the birth of stars
- precursor material for the formation of planets
- hides astronomical objects from our view

Interstellar observations are crucial to understanding the origins of the universe

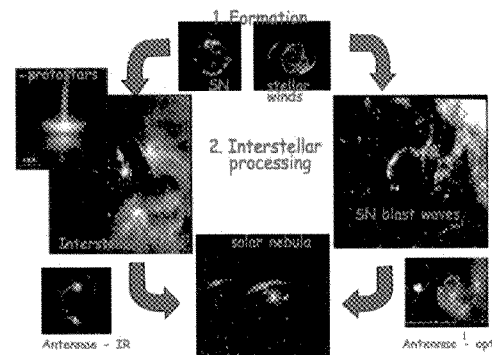


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The importance of studying silicates

Spectral features attributed to:

- silicates
- carbonaceous grains
- PAHs

↳ inferences on chemical and physical structure

Their spectra need be analyzed through laboratory experiments reproducing astrophysical environments (See Henning & Mutschke, 2010)

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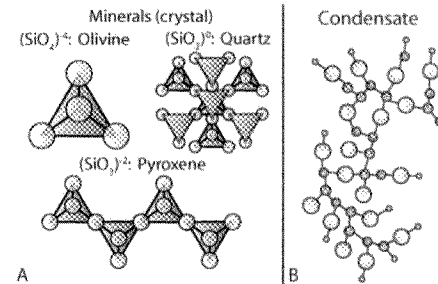


Figure: A) Silicates on Earth are ordered solids. B) In space their structure is chaotic. (Adapted from Rinehart et al., 2008)

The optical constants as primary parameters

Definition

Complex refractive index $m = n + ik$

- The refractive index n determines the velocity of constant-phase waves.
- The extinction index k determines the attenuation of the wave as it propagates through the medium.

Dielectric constant $\epsilon = (n + ik)^2 = \epsilon' + i\epsilon''$

→ In fact, the optical constants are not directly comparable

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Remark: the optical constants are not directly measurable

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Objectives of the OPASI-T program

- Experimental apparatus and measurements

- Development of a dedicated code for the computation of the optical constants as a function of wavelength and temperature
- Validation through application to known materials
- Analysis and interpretation of post-processed data
- Population of a library of optical properties in the far infrared regime

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Hypotheses and mathematical models

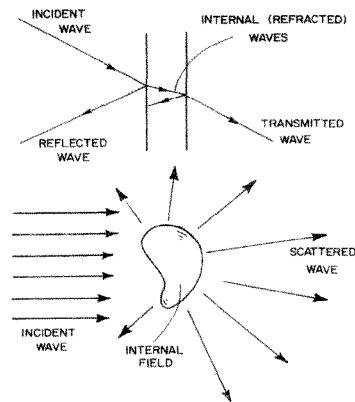


Figure: Analogy between scattering by a particle and transmission-reflection-absorption by a slab (Bohren and Huffman, 1983)

Transmission-line approximation

- One-layer slab model (Bohren and Huffman, 1983)
- Beer's law (Hulst et al., 1986)

Transition modes

- Lorentz model

Mixtures

- Maxwell Garnett formula (Maxwell Garnett, 1904)

Hypotheses and mathematical models

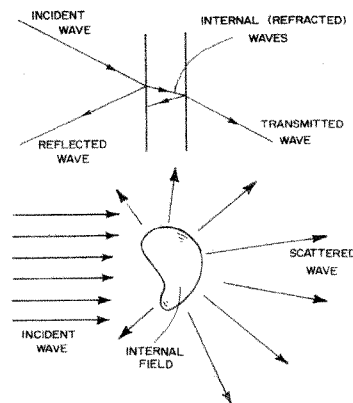


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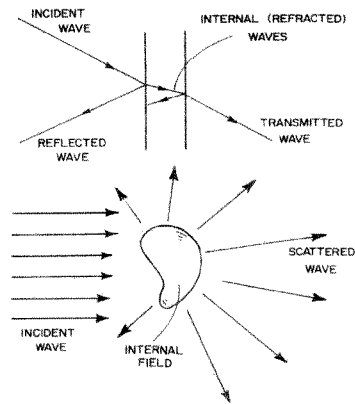


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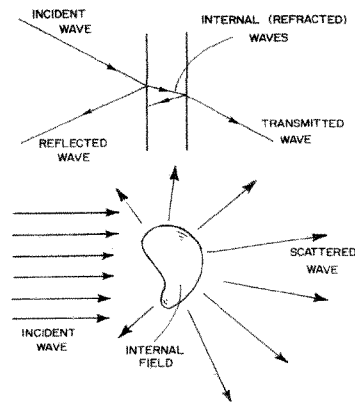


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Constrained minimization as main working tool

Definition (Least-Squares Nonlinear Fit)

$$\min_{DOFs} \chi_m^2 = \min_{DOFs} \frac{1}{N} \sum_{j=1}^N [T(DOFs, \lambda_j) - T_{measured}]^2$$

$$DOF_{min} \leq DOF \leq DOF_{max}$$

N = number of data points

λ = wavelength

Initial condition \rightarrow Fit \rightarrow DOFs \rightarrow $\begin{cases} I, R, A \\ \alpha, k, \dots \end{cases}$

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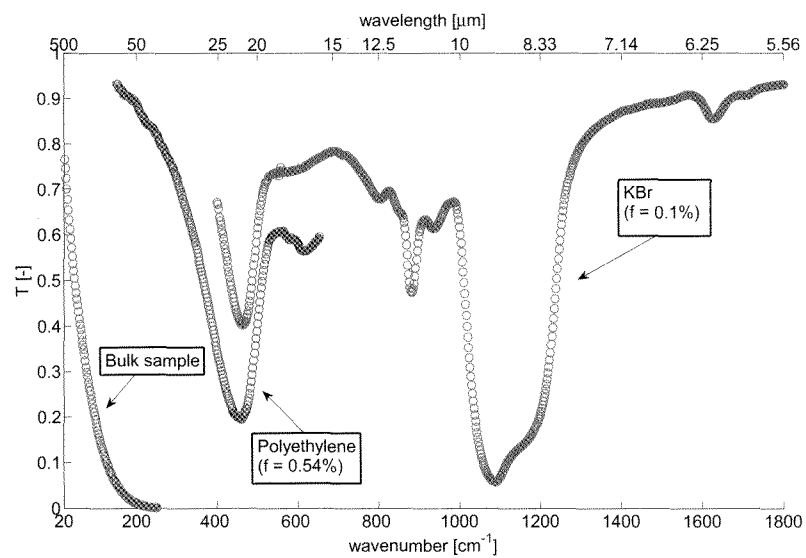
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$$\text{Initial condition} \rightarrow \text{Fit} \rightarrow DOFs \rightarrow \begin{cases} T, R, A \\ n, k, \varepsilon \end{cases} \forall \lambda_j$$

SiO_x : Measured transmission spectrum at room temperature



SiO_x : Sample characterization

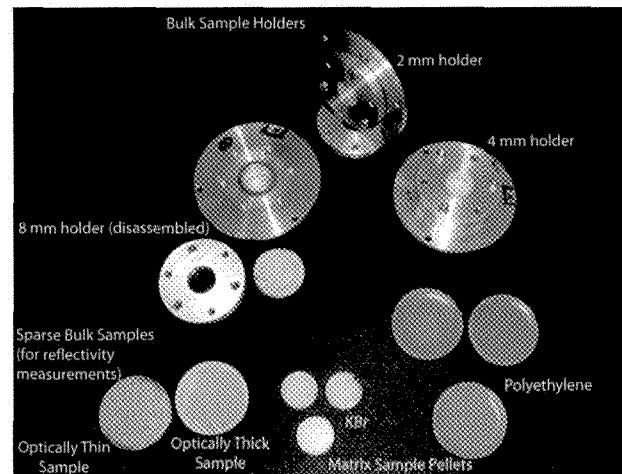


Figure: Various sample preparations are needed to cover the wide frequency range (Rinehart, Cataldo, et al., *Applied Optics*, in press).

SiO_x : Sample characterization

Each sample preparation has a different optical depth, which allows us to obtain transmission values in the range of 0.2-0.8 as needed to determine the optical constants to high accuracy.

Sample type	Spectral coverage [μm]
8-mm	300 – 1000
4-mm	100 – 500
2-mm	100 – 350
Polyethylene	15 – 100
KBr	1 – 25

SiO_x : How to extract the optical constants (bulk samples)

Beer's law

$$T = (1 - R)^2 \exp(-\alpha h)$$

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$\alpha = a \left(\frac{\omega}{2\pi} \right)^b$$

h = sample thickness

$$k = \frac{\alpha}{2\omega} = \frac{a}{2\omega} \left(\frac{\omega}{2\pi} \right)^{b-1}$$

$$T = T(n, a, b)$$

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SiO_x : How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{\text{eff}} = \varepsilon_{\text{eff}}(f, \varepsilon_b, \varepsilon_i)$$

$$f = (n - 1)^2 / (n^2 + 2)^2 \times \sum_{i=1}^N \frac{\varepsilon_i - \varepsilon_b}{\varepsilon_i + 2\varepsilon_b} \times \frac{f_i}{1 - f_i}$$

$$n = n(f, \varepsilon_b, \text{DOF}_1, \dots)$$

$$T = T(f, \varepsilon_b, \text{DOF}_1, \dots)$$

SiO_x : How to extract the optical constants (mixtures)

Maxwell-Garnett formula

$$\varepsilon_{eff} = \varepsilon_{eff}(f, \varepsilon_b, \varepsilon_i)$$

Lorentz model

$$\varepsilon_i = (n + ik)^2 = \varepsilon_{i,\infty} + \sum_{j=1}^M b_m \frac{\omega_{pj}^2}{\omega_{0j}^2 - \omega^2 - i\omega\nu_j} = \varepsilon_i(DOFs, \omega)$$

$$n(\omega) = \sqrt{\varepsilon_r(\omega)/4\pi} = \sqrt{\varepsilon_i(DOFs, \omega)/4\pi}$$

$$k(\omega) = \sqrt{\varepsilon_i(DOFs, \omega)/4\pi}$$

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Modified Lorentz model (Sihvola, 1999)

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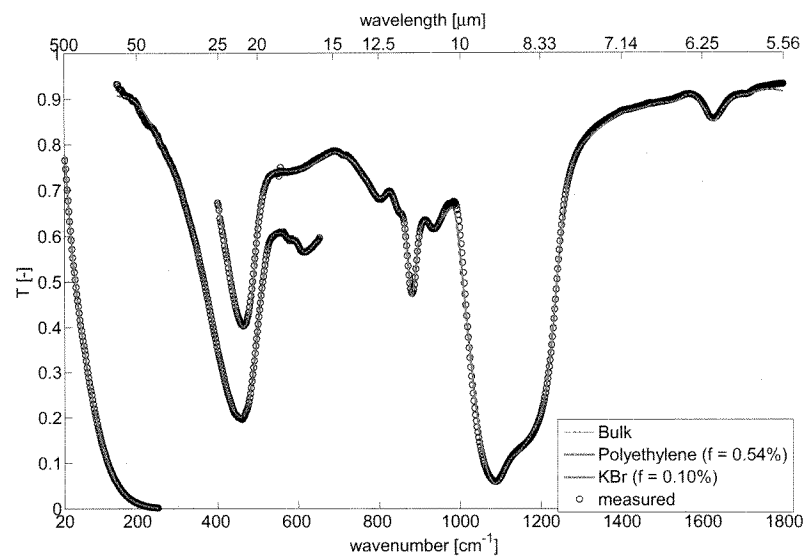
Modified Lorentz model (Sihvola, 1999)

$$\varepsilon_{eff} = \varepsilon_{eff}(f, \varepsilon_b, DOFs_i, \omega)$$

One-layer slab model (averaged)

$$T = T[f, \varepsilon_b, (4M + 1)DOFs_i, \omega]$$

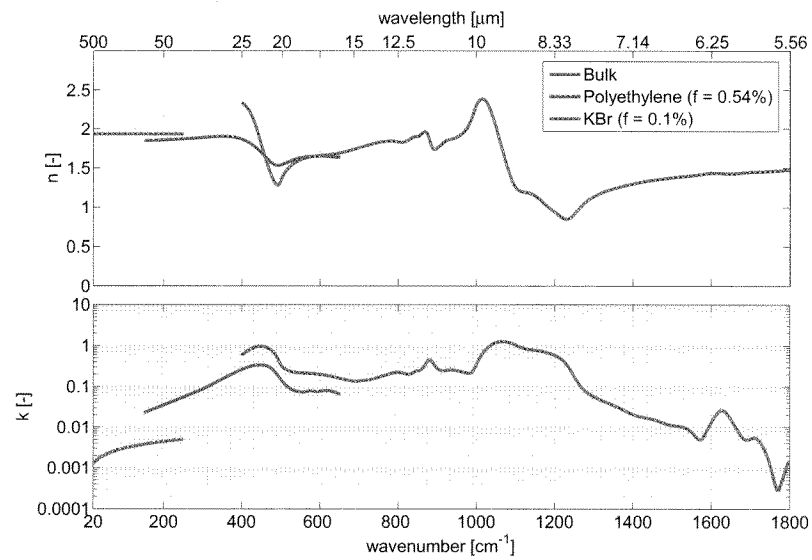
SiO_x : Fit and output parameters (Cataldo et al., in prep.)



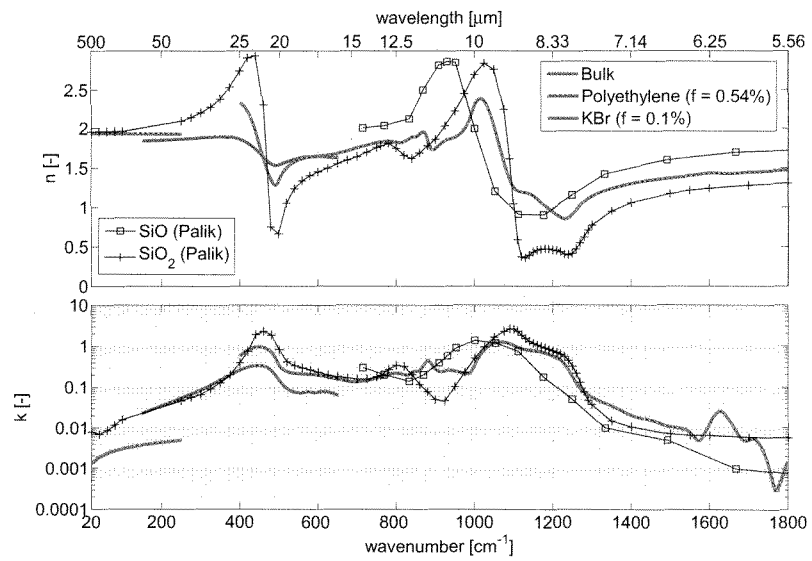
SiO_x: Fit and output parameters

		Bulk (4-mm)	Polyethylene	KBr
DOFs		3	53 (13 LOs)	153 (38 LOs)
Residual	average	0.32	0.62	0.25
ΔT [%]	maximum	2.68	3.93	1.47
χ_m^2		$2.55 \cdot 10^{-5}$	$11.12 \cdot 10^{-5}$	$1.29 \cdot 10^{-5}$
σ		0.005	0.012	0.008
χ^2		109.89	239.81	146.26
χ_ν^2		0.93	1.15	0.25

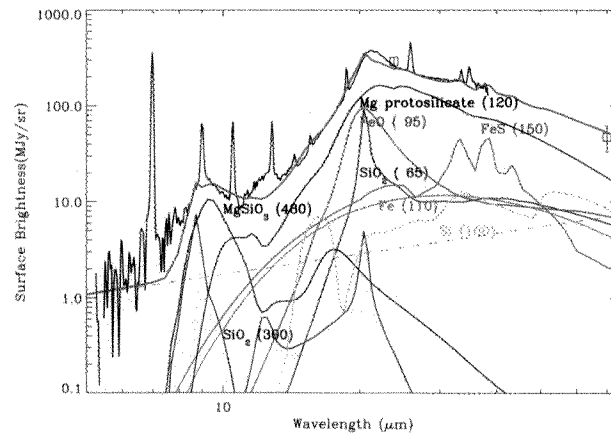
SiO_x : The optical constants in the FIR and MIR



SiO_x : The optical constants in the FIR and MIR





SiO_x : The optical constants in the FIR and MIR



(Adapted from Rho et al., 2008)

Our sample description

	Advantages	Disadvantages
Bulk sample	n consistent with other measurements	n not well constrained
	$a = 0.003$, $b = 1.552$ (Agladze et al., 95;...)	Need for data at longer wavelengths
Mixture	$n - k$ independent from filling fraction 	$n - k$ dependent on matrix
	$x \approx 1.5$	Fine-tuning
	DOFs well constrained	of starting guess
	Outputs for mix and particles 	Uncertainty in measurements

Next steps

- Measured reflectance data (TOP PRIORITY)
 - Amorphous dependence (Cataldo et al., in prep.)
 - Development of more sophisticated models
 - Realistic porous powders (Fe and Mg-rich silicates (Kunze, Cataldo et al., in prep.))
 - Heterogeneity
 - Multiple-layered structures
 - Unparalleled facets and roughness
- Application to new upcoming laboratory data and observations

Next steps

- Measured reflectance data (TOP PRIORITY)
- Temperature dependence (Cataldo et al., in prep.)
- Development of more sophisticated models
 - Better mineral providers: Fe- and Mg-rich silicates (Kluze, Cataldo et al., in prep.)
 - Anisotropy
 - Multiple-layered structures
 - Unparallelled faces and roughness
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Next steps

- Measured reflectance data (TOP PRIORITY)
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 - Metal-enriched powders: Fe- and Mg-rich silicates (Kinzer, Cataldo, et al., in prep.)
 - Scattering
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 - Unparalleled faces and roughness

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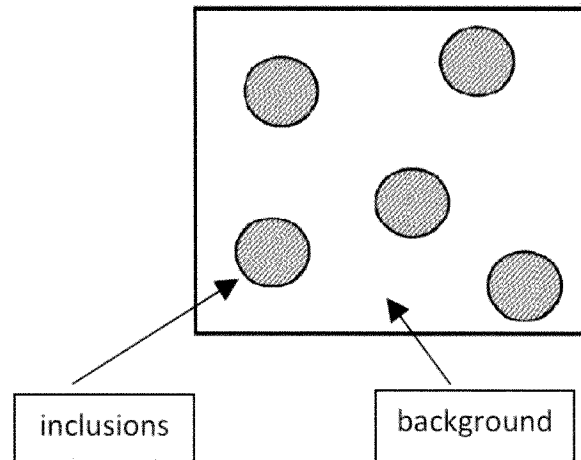
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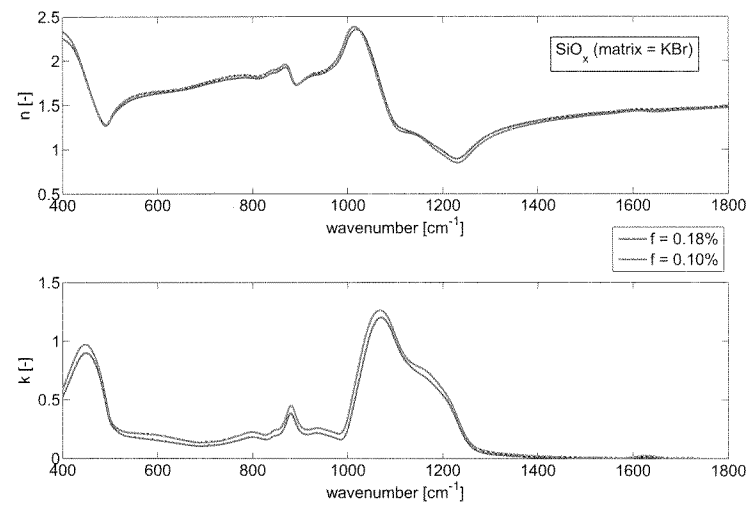
Thanks!
Questions?

The effective medium structure

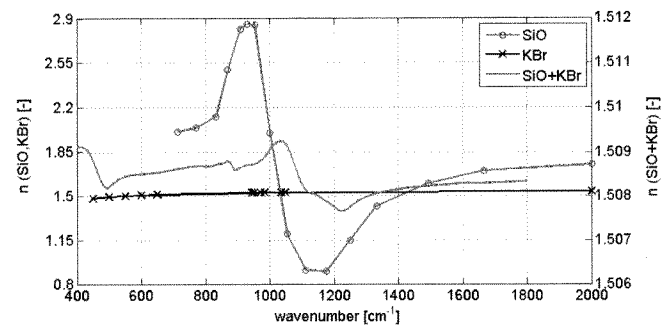
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The optical constants as a function of filling fraction



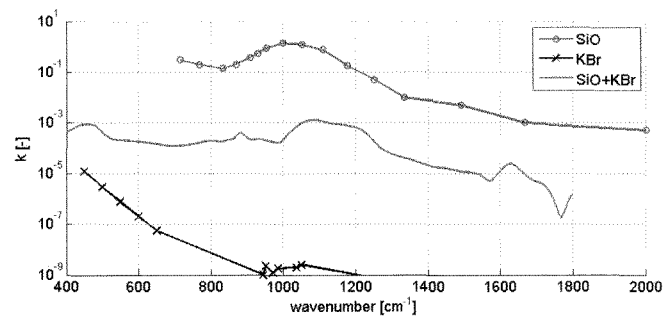
The optical constants for the $SiO_x - KBr$ mixture



(Rinehart, Cataldo, et al., *Applied Optics*, in press)

The optical constants for the $\text{SiO}_x - \text{KBr}$ mixture

Back

(Rinehart, Cataldo, et al., *Applied Optics*, in press)